

Role of band mixing on superconductivity in two-dimensional system

K. Sengupta and S. K. Ghatak
Dept. of Physics & Meteorology,
I. I. T., Kharagpur-721302

Assuming that the p-states of O are involved in superconductivity in oxide superconductor and using the BCS approximation to the pairing interaction we examine the effect of the mixing between the p-orbital of O and d-orbital of Cu on superconductivity. It is found that superconductivity vanishes beyond a critical value of hybridization (V_c) that depends on charge transfer energy gap. Hybridization induces a pairing correlation $f_d = \langle d_{-k\downarrow} d_{k\uparrow} \rangle$ between d-electrons and it vanishes at $V=0$ and V_c passing through a maximum. The ratio (Δ_0/T_c) deviates from the BCS value before it goes to zero at V_c .

Key Words : Superconductor, Hybridization

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It is now well documented that the Cu-O square-lattice planes which are present in all high T_c systems play dominant role in determining the properties of normal as well as superconducting states [1-4]. The electronic structure of Cu-O layer can be described by two-band model and hybridization between p-states of O and d-states of Cu replaces the van Hove singularity in density of states of uncoupled system by a peak [5]. It is expected that the superconducting state will be influenced by band mixing. The superconductivity in

two band model without mixing has been studied earlier [6-9]. The effect of logarithmic divergence in DOS on superconductivity in these systems has been considered based on one band model [10-12]. The effect of mixing on superconductivity in two-band model has been examined assuming pairing in narrow band and constant DOS around E_F [13]. Here we present some results of a model study on the effect of mixing and logarithmic variation of DOS near E_F on superconductivity based on two-band model.

We consider two overlapping bands :one narrow band (d-like) and other wide band (p-like) and the pairing interaction between the p-electrons. The model is described by the Hamiltonian,

$$H = \sum_{k,\sigma} E_{dk} d_{k\sigma}^\dagger d_{k\sigma} + \sum_{k,\sigma} E_{pk} p_{k\sigma}^\dagger p_{k\sigma} + \sum_{k,\sigma} V_k (d_{k\sigma} p_{k\sigma}^\dagger + \text{h.c.}) - G \sum_{k,l} p_{k\uparrow}^\dagger p_{-k\downarrow}^\dagger p_{-l\downarrow} p_{l\uparrow}$$

The first two terms represent respectively a narrow d-band with energy E_{dk} and a wide p-band with energy E_{pk} . Hybridization between the bands (third term) represents hopping of electrons from Cu site to adjacent O site and vice-versa. The last term is the BCS pairing interaction between p-electrons. The interaction is finite within a characteristic energy interval ω_0 about Fermi level E_F . For phononic mechanism, ω_0 is the Debye energy. It is convenient to use the Green's function approach to obtain anomalous correlation functions $\langle p_{-k\downarrow} p_{k\uparrow} \rangle$ and $\langle d_{-k\downarrow} d_{k\uparrow} \rangle$. Using the BCS

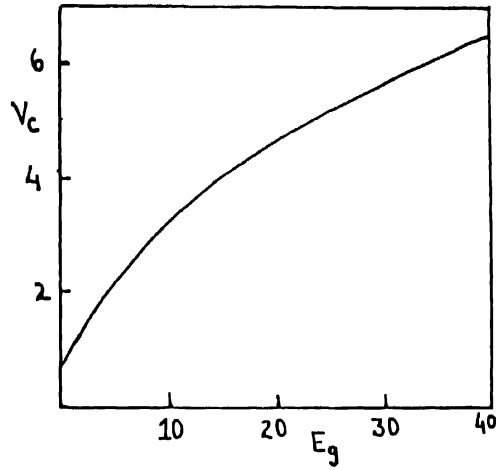
approximation we obtain the matrix equation for different Green's functions

$$\begin{bmatrix} E-E_{pk} & V_k & 0 & \Delta \\ V_k & E-E_{dk} & 0 & 0 \\ 0 & 0 & E+E_{pk} & V_k \\ \Delta & 0 & V_k & E+E_{dk} \end{bmatrix} \begin{pmatrix} \epsilon_{pp} \\ \epsilon_{dp} \\ h_{dp} \\ f_{pp} \end{pmatrix} \text{ or } \begin{pmatrix} \epsilon_{pd} \\ \epsilon_{dd} \\ f_{dd} \\ h_{pd} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad (1)$$

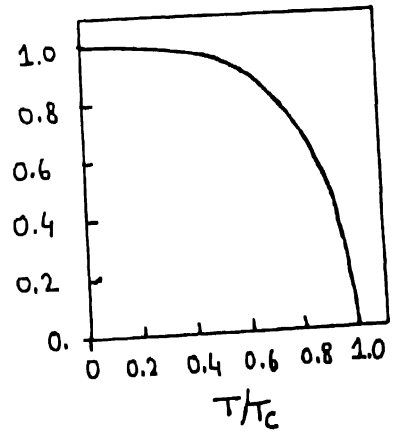
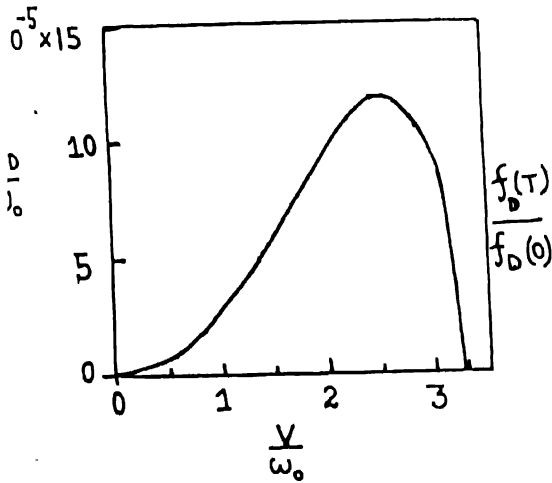
where $\epsilon_{pp} = \langle\langle p_{k\uparrow}; p_{k\sigma}^{\dagger} \rangle\rangle$, $\epsilon_{dp} = \langle\langle d_{k\sigma}; p_{k\sigma}^{\dagger} \rangle\rangle$, $h_{dp} = \langle\langle d_{-k\sigma}^{\dagger}; p_{k\sigma}^{\dagger} \rangle\rangle$, $f_{pp} = \langle\langle p_{-k\sigma}; p_{k\sigma}^{\dagger} \rangle\rangle$ and Green's function in second column matrix are obtained from corresponding element, of first column by interchanging p and d. The gap parameter $\Delta = \sum_k' G \langle p_{-k\downarrow} p_{k\uparrow} \rangle$ where prime in the sum indicates that only states lying within the Debye energy interval about E_F should be considered. The eqns. for Δ and $f_d = \sum_k' \langle d_{-k\downarrow} d_{k\uparrow} \rangle$ can be obtained from eqn.(1) [14] and are solved numerically.

Considering local symmetry of Cu-O layer, we take the homothetic relation between energy dispersion of p- and d- bands $E_{dk} = E_g + \alpha E_{pk}$ where parameter α determines effective mass of d-electron and E_g is charge transfer energy gap. The density of state (DOS) for p-band close to the Van Hove singularity is modelled as [11] $N(E) = (1/2W) \ln |W/E|$. As the pairing occurs within the small energy interval about E_F , we neglect dispersion of V_k assumes $V_k = V$. The results are given with input parameters $G/W = 0.1$, $W = 100\omega_0$, $\alpha = 0.1$ and $E_F = 0$ and varying V and E_g . In the

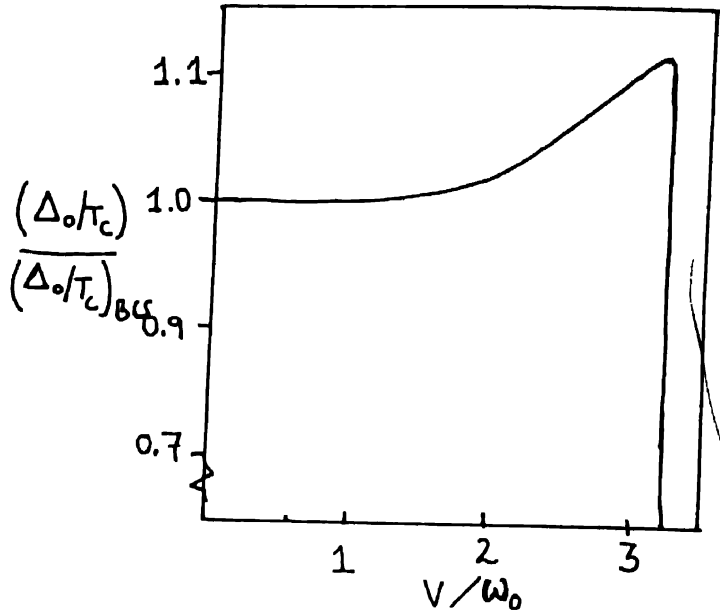
following all energy parameters are expressed in terms of ω_0 . It is observed that the superconducting transition temperature T_c is diminished in presence of mixing and T_c vanishes beyond a critical value of hybridization. This critical value V_c is smallest for resonating bands ($E_g=0$) and increases with the increases of E_g (Fig.1). The phase diagram and thermal behaviour of Δ with V are reported earlier [14]. The pairing correlation f_d at $T=0$ is zero at $V=0$ and V_c (Fig.2a). For small V it increases quadratically with V and attains a maximum for $V < V_c$. Near V_c it approaches to zero sharply. The temperature dependence of f_d is dominated by that of gap parameter Δ as is evident from reduced plot $f_d(T)/f_d(0)$ Vs T/T_c (Fig.2b). The effect of mixing on the ratio (Δ_0/T_c) is small for small V (Fig.3). However, it increases compared to the BCS value for V close to V_c before it goes to zero at V_c . Hybridization acts as a pairing breaking interaction as there is no pairing interaction in d-band. On the other hand, it can enhance tendency of pairing if some correlation between up- and down - d-electrons exists. Valence fluctuating systems rarely exhibits superconducting state although they have large electron-phonon interaction and large DOS at E_F . This may be due to large hybridization between localized f- and band- states. Induced correlation will play an important role in



1. Plot of critical Value V_c against E_g . Parameters are $G=10, W=100, E_F=0$ & $\alpha=0.1$ with $\omega_n=1$.



2.a) Pairing correlation f_d at $T=0$ Vs V and
 b) Reduced correlation $f_d(T)/f_d(0)$ Vs T/T_c for $E_g=1$. Other parameters are same as in Fig.1.



3. Variation of ratio of (Δ_0/T_c) to (Δ_0/T_c) of BCS with hybridization V for above parameters.

competition between antiferromagnetism and superconducting states in high- T_c system.

References

- [1] V.J. Emery, Phys. Rev. Lett. 50, 2794 (1987)
- [2] H. Chi & A.D.S. Nagi, Phys. Rev. D46 421 (1992)
- [3] D.M. Newns, P. Pattanaik and C.C. Tseui Phys. Rev., B 43 3075 (1991)
- [4] D.M. Eagles & N. Savvides, Physica C150 250 (1989)
- [5] S. Basu & S.K. Ghatak, (unpublished)
- [6] H. Suhl, B.T. Matthias & L.R. Walker Phys. Rev. Lett. 3 351 (1959)
- [7] J. Kondo, Prog. Theo. Phys. 29 1 (1963)
- [8] J. Ziehlinski & P. Zawadzki, Z. Phys. B47 35 (1988)
- [9] B.K. Chakraverty, Phys. Rev. B40 4047 (1993)
- [10] J.M. Getino, H. Rubio & M. de Llano Solid State Comm. 83 831 (1992)
- [11] C.C. Tsuei, Physica A160 230 (1990)
- [12] J. Friedel, J. Phys. Condens. Matter 1 1757 (1989)
- [13] J. Labbe & J. Bok, Europhys. Lett 3 1225 (1987)
- [14] F. Yndurain, Solid State Comm. 81 939 (1992)
- [15] M. Jopliassn, M.A. Contino, A. Troper Phys. Rev. B45 2906 (1992)
- [16] K. Sengupta & S.K. Ghatak Phy. Lett. A186 419 (1994)